

data using the program DINA and the supporting programs CALIBA,  
HABAS and GLOMSA. *J. Mol. Biol.* 217:517-530, 1991.

- 5
14. Bernstein, F. C., Koetzle, T. F., Williams, G. J. B., Meyer Jr., E. F., Brice, M. D., Rodgers, J. R., Kennard, O., Simanouchi, T., Tasumi, M. The protein data bank: a computer-based archival file for macromolecular structures. *J. Mol. Biol.* 112:535-542, 1977.
15. Kolinski, A., Skolnick, J. Monte Carlo simulations of protein folding. I. Lattice model and interaction scheme. *Proteins* 18:338-352, 1994.
- 10
16. Kolinski, A., Skolnick, J. "Lattice Models of Protein Folding, Dynamics and Thermodynamics." Austin, TX: R. G. Landes Co., 1996.
17. Kolinski, A., Skolnick, J. Parameters of statistical potentials. Available by ftp from public directory scripps/edu(pub/andr/side\_only/\*). 1997.
- 15
18. Godzik, A., Skolnick, J., Kolinski, A. Regularities in interaction patterns of globular proteins. *Protein Eng.* 6:801-810, 1993.
19. Kyte, J., Doolittle, R. F. A simple method for displaying the hydrophatic character of protein. *J. Mol. Biol.* 157:105-132, 1982.
20. Skolnick, J., Jaroszewski, L., Kolinski, A., Godzik, A. Derivation and testing of pair potentials for protein folding. when is the quasichemical approximation correct? *Protein Sci.* 6:676-688, 1997.
- 20
21. Kolinski, A., Godzik, A., Skolnick, J. A general method for the prediction of the three dimensional structure and folding pathway of globular proteins. Application to designed helical proteins. *J. Chem. Phys.* 98:7420-7433, 1993.
22. de Gennes, P. G., "Scaling Concepts in Polymer Physics." Ithaca, NY; Cornell University Press, 1979.
- 25
23. Kolinski, A., Skolnick, J., Determinants of secondary structure of polypeptide chains: Interplay between short range and burial interactions. *J. Chem. Phys.* 107:953-964, 1997.
24. Eisenberg, D., McLachlan, A. D., Solvation energy in protein folding and binding. *Nature* 319:199-203, 1986.
- 30
25. Godzik, A., Kolinski, A., Skolnick, J., Are proteins ideal mixtures of amino acids? Analysis of energy parameter sets. *Protein Sci.* 4:2107-2117, 1995.

26. Godzik, A., Knowledge-based potential for protein folding: What can we learn from known structures? *Curr. Biol.* 4:363-366, 1996.
27. Kolinski, A., Jaroszewski, L., Rotkiewicz, P., Skolnick, J., An efficient Monte Carlo model of protein chains. Modeling the short-range correlations between side group centers of mass. *J. Phys. Chem.* 102:4628-4637, 1998.
28. Kolinski, A., Skolnick, J., Monte Carlo simulations of protein folding. II. Application to protein A, ROP, and crambin. *Proteins* 18:353-366, 1994.
29. Kolinski, A., Galazka, W., Skolnick, J., Computer design of idealized  $\beta$ -motifs. *J. Chem. Phys.* 103:10286-10297, 1995.
30. Kolinski, A., Milik, M., Rycobel, J., Skolnick, J., A reduced model of short range interactions in polypeptide chains. *J. Chem. Phys.* 103:4312-4323, 1995.
31. Kolinski, A., Galazka, W., Skolnick, J., On the origin of the cooperativity of protein folding. Implications from model simulations. *Proteins* 26:271-287, 1996.
32. Olszewski, K., Kolinski, A., Skolnick, J., Does a backwardly read protein sequence have a unique native state? *Protein Eng.* 9:5-14, 1996.
33. Diszewski, K., Kolinski, A., Skolnick, J., Folding simulations and computer redesign of protein  $\alpha$  three-helix bundle motifs. *Proteins* 25:286-299, 1996.
34. Ortiz, A. R., Hu, W. P., Kolinski, A., Skolnick, J., A method for prediction of the tertiary structure of small proteins. *J. Mol. Graph.* in press.
35. Ortiz, A. R., Hu, W. P., Kolinski, A., Skolnick, J., Method for low resolution prediction of small protein tertiary structure. In: "Proceedings of the Pacific Symposium on Biocomputing '97." Altman, R. B., Dunker, A. K., Hunter, L., Klein, T. E. (eds.), Singapore: World Scientific Pub., 1997 316-327.
36. Skolnick, J., Kolinski, A., Monte Carlo lattice dynamics and the prediction of protein folds. In: "Computer Simulations of the Biomolecular Systems. Theoretical and Experimental Studies," van Gunsteren, W. F., Weiner, P. K., Wilkinson, A. J. (eds.). The Netherlands: ESCOM Science Pub. 395-429, 1997.
37. Kabsch, W., Sander, C., Dictionary of protein secondary structure: Pattern recognition of hydrogen-bonded and geometrical features. *Biopolymers* 22:2577-2637, 1983.

- 5 38. Binder, K., "Monte Carlo Methods in Statistical Physics." Berlin: Springer-Verlag, 1986.
39. Skolnick, J., Kolinski, A., Protein modelling. In: "Encyclopedia of Computational Chemistry," Schleyer, P., Kollman, P. (eds.). Sussex, England: John Wiley & Sons, in press.
40. Richardson, J., The anatomy and taxonomy of protein structure. *Adv. Protein Chem.* **34**:167-339, 1981.
- 10 41. Gronenborn, A., Filpula, D. R., Essig, N. Z., Achari, A., Whitlow, M., Wingfield, P. T., Clore, G. M., A novel highly stable fold of the immunoglobulin binding domain of streptococcal protein. *G. Science* **253**:657-660, 1991.
42. Koradi, R., MOLMOL: A program for display and analysis of macromolecular structures. *J. Mol. Graph.* **14**:51-55, 1996.
- 15 43. Goebel, U., Sander, C., Schneider, R., Valencia, A., Correlated mutations and residue contacts in proteins. *Proteins* **18**:309-317, 1994.
44. Kolinski, Method for improvement of threading models, *Proteins* **37**:592-610, 1999.

20

25

30